

Analytical Expressions for a Hyperspherical Adiabatic Basis Three Particles in 2 Dimensions

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ABSTRACT

For a particular case of three-body scattering in 2 dimensions, we demonstrate analytically that the behaviour of the adiabatic potential is different from that of the hyperspherical coupling matrix elements, thereby leading to a phase shift that tends to zero, as the energy goes to zero, instead of to a constant. We consider two particles interacting with binary repulsive step potentials, one acting as a spectator, and solve analytically for the adiabatic eigenvalues and eigenvectors, for all values of ρ . We are thereby able to obtain the leading terms in the long range behaviour of the effective potentials, and confirm its inverse logarithmic nature, suggested from a previous numerical study.

Introduction

In a previous paper[1], the authors show how, starting from hyperspherical harmonic expansions, they obtained adiabatic potentials, suitable for the calculations of three-body phase shifts at low energies. The calculations were for 3 particles in a plane, subject to finite repulsive core interactions.

The calculations were meant to establish a method which would lead to the evaluation, at low temperature, of a third fugacity coefficient in Statistical Mechanics. The latter task was subsequently carried out by Jei Zhen and one of the authors[2]. In both investigations, it was important to consider different cases, corresponding to the distinct representations of the permutation group and different physical situations, with either the 3 particles interacting or simply two of them interacting, with the third acting as a spectator.

Absolutely crucial, in these investigations, is the large- ρ behaviour of the adiabatic potentials. The nature of the long “tail” of the adiabatic potential determines how the correspondent eigenphase shift behaves, as the energy tends to zero. Thus, our most significant result was that for the 3 most important types of the phase shifts, associated with the cases of ${}^0\Gamma_{1g}$, ${}^0\Gamma_{2g}$ and $\bar{\delta}$, the adiabatic potentials (the adiabatic eigenvalue minus a centrifugal term) behave as $1/(\rho^2 \ln \rho)$, for large values of ρ , instead of the $1/\rho^2$ of the hyperspherical potential matrix elements. This then implies that the phase shifts, instead of tending to constants as the energy goes to zero, behave as $1/(\ln q)^2$, and therefore go to zero! (The variables ρ and q are, respectively, the hyper radius and the reduced wave number.)

Though, in our old paper, our basic material was numerical, we were able nevertheless to propose “heuristic” formulae, to characterize the asymptotic behaviour of the 3 types of eigenpotentials, of the remodeling that takes place to yield a different scattering from the one expected from the solution of a finite number of hyperspherical equations.

In this paper, we present analytical results, where we show that in one of the three cases mentioned above, the case $\bar{\delta}$, we succeeded in calculating analytically the adiabatic eigenvectors and eigenvalues for all the values of ρ , and therefore also in the asymptotic region.

While this calculation involves a case where only two of the particles interact, while the 3rd particle acts as a spectator, it is well to note that in the hyperspherical coordinate system the two-body interaction is long ranged (in ρ) and also that in the full hyperspherical calculations of the other cases, we only need, using symmetry and enforcing a restriction on the quantum numbers, to take into account the matrix element of one of the pair potentials.

Here, then, our calculations allow us to re-examine our previous results, and confirm and extend the asymptotic form (and coefficients) that can be used to characterize the long range behaviour of the adiabatic potentials.

The KL Hyperspherical Coordinate System

The Harmonic Basis

For a system of three equal mass particles in two dimensions, we define the Jacobi coordinates

$$\vec{\eta} = (\vec{r}_1 - \vec{r}_2)/\sqrt{2} \quad \text{and} \quad \vec{\xi} = \sqrt{2/3}(\frac{\vec{r}_1 + \vec{r}_2}{2} - \vec{r}_3),$$

which allows us to separate, in the Hamiltonian, the center of mass coordinates from those associated with the internal motion.

Kilpatrick and Larsen[3] then introduce hyperspherical coordinates, associated with the moment of inertia ellipsoid, of the 3 particles, which allows them to disentangle permutations from rotations and obtain harmonics which are pure representations of both the permutation and the rotation group. Taking the z axis normal to the plane of the masses, we write for the cartesian components of the Jacobi coordinates

$$\begin{aligned} \eta_x &= \rho(\cos \vartheta \cos \varphi \cos \psi + \sin \vartheta \sin \varphi \sin \psi), \\ \eta_y &= \rho(\cos \vartheta \cos \varphi \sin \psi - \sin \vartheta \sin \varphi \cos \psi), \\ \xi_x &= \rho(\cos \vartheta \sin \varphi \cos \psi - \sin \vartheta \cos \varphi \sin \psi), \\ \xi_y &= \rho(\cos \vartheta \sin \varphi \sin \psi + \sin \vartheta \cos \varphi \cos \psi), \end{aligned} \tag{1}$$

in terms of the hyper radius ρ and of the three angles ϑ , φ and ψ .

The harmonics, in their unsymmetrized form, are then

$$Y_N^{\nu\lambda}(\Omega) = C_n^{\alpha\beta} \Theta_n^{\alpha\beta}(x) e^{i\nu\varphi} e^{i\lambda\psi} \tag{2}$$

where $x = \sin 2\vartheta$ and

$$\Theta_n^{\alpha\beta}(x) = (1-x)^{\alpha/2} (1+x)^{\beta/2} P_n^{\alpha,\beta}(x) \tag{3}$$

$P_n^{\alpha,\beta}(x)$ is a Jacobi polynomial, and the normalization constant is

$$C_n^{\alpha\beta} = \left\{ \left(\frac{N+1}{2^{\alpha+\beta+1}} \right) \binom{n+\alpha+\beta}{\alpha} \binom{n+\alpha}{\alpha}^{-1} \right\}^{1/2}.$$

The hyper radius ρ satisfies $\rho^2 = \eta^2 + \xi^2$ and the angular components have the ranges

$$-1 \leq x \leq 1, \quad -\pi/2 \leq \varphi \leq \pi/2, \quad 0 \leq \psi \leq 2\pi.$$

Finally we have for the indices the relations

$$n = \frac{1}{2}[N - \max\{|\nu|, |\lambda|\}], \quad \alpha = \frac{1}{2}|\nu + \lambda|, \quad \beta = \frac{1}{2}|\nu - \lambda|,$$

where N is the degree of the harmonic, and λ is the inplane angular momentum quantum number. The indices ν and λ take on the values $-N$ to N in steps of 2; all three have the same parity and $N = 0, 1, 2, \dots$

Linear combinations of the basic harmonics can then be formed[3] to obtain irreducible bases, adapted to the symmetries of the physical problems[1, 2].

The Adiabatic Basis

For our model, the particles interact via a binary step potential

$$V(r_{ij}) = \begin{cases} V_0, & r_{ij} \leq \sigma \\ 0, & r_{ij} > \sigma \end{cases} \quad (4)$$

where the height V_0 , and the range, σ , are both finite.

The adiabatic eigenfunctions B_l are then defined as satisfying

$$\left\{ -\frac{1}{\rho^2} \nabla_{\Omega}^2 + \frac{2m}{\hbar^2} V(\rho, \Omega) \right\} B_l = \lambda_l(\rho) B_l, \quad (5)$$

where $V(\rho, \Omega)$ is either the sum of the binary potentials or, simply one of the binary potentials, say $V(r_{12})$, expressed as a function of ρ and the angles. The index l stands for the set of quantum numbers which characterize and index the particular class of solutions. $\lambda_l(\rho)$ is the eigenvalue, which upon subtraction of a “centrifugal” type term yields the effective potential, of concern to us later on.

The eigenfunctions may now be used to expand the wavefunctions of the physical systems:

$$\Psi = \sum_{\nu} B_{\nu}(\rho, \Omega) \phi_{\nu}(\rho), \quad (6)$$

where the amplitudes $\phi_l(\rho)$ are the solutions of the coupled equations:

$$-\sum_{\nu} \int d\Omega B_l^*(\Omega, \rho) \frac{\partial^2}{\partial \rho^2} (B_{\nu}(\Omega, \rho) \phi_{\nu}(\rho)) + \lambda_l(\rho) \phi_l(\rho) = (2mE/\hbar^2) \phi_l(\rho). \quad (7)$$

The adiabatic eigenfunctions can themselves be expanded in hyperspherical harmonics and this is how a large set of them were calculated in the papers quoted earlier. The symmetries of the hyperspherical harmonic basis are, of course, reflected in the solutions of the adiabatic eigenvectors. For the fully symmetric Hamiltonian, the set of solutions divides into nine separate subsets[2], each requiring calculations involving combinations of matrix elements of only one of the binary potentials, but with restrictions on the quantum numbers of the unsymmetrized harmonics involved. In the case of two interacting particles, with a third as a spectator, we find an additional four subsets.

The numerical approach was then, for each ρ , to evaluate a large potential matrix, with the appropriate harmonic basis, add to this the (diagonal) “centrifugal” contribution arising from the angular part of the kinetic energy (the angular part of the Laplacian in the Hamiltonian) and diagonalize to obtain the required adiabatic eigenvalues. The number of harmonics, needed for numerical convergence, increases as a function of ρ , but it was our fortunate experience to find that it was possible to evaluate correctly the eigenvalues, that we sought, for values of ρ large enough that the behaviour of $\lambda_l(\rho)$ could be described by asymptotic forms. We were able to characterize them, and this gave us the values of $\lambda_l(\rho)$ for all the larger values of ρ .

Dual Polar Set of Coordinates

The Harmonic Basis

In this part of the paper we wish, exclusively, to consider the case of two particles interacting together, the third acting as a spectator. As we shall show, we are then able to obtain exact adiabatic solutions.

Our reasoning is as follows. When the third particle does not interact with the other two, this must imply that the motion of the pair (1,2), and therefore its angular momentum, is unaffected by the motion of the third particle. In a parallel fashion, the motion of the third particle, and its angular momentum about the center of mass of the particles (1,2), must be a constant as well. If we choose our coordinates carefully, the angular behaviour of two of the angles should “factor” out and, for a given ρ , only one variable should be involved in a key differential equation.

We note that in the KL coordinates, the distances between particles involve two of the angles, for example r_{12}^2 equals $\rho^2(1 + \cos 2\vartheta \cos 2\varphi)$. To get around this, we choose an angle to give us the ratio of the length of the 2 Jacobi vectors, and then polar coordinates for each of them. Thus, we represent Ω by $(\theta_1, \theta_2, \phi)$, where $\eta = \rho \cos \phi$, $\xi = \rho \sin \phi$ and $\eta_x = \eta \cos \theta_1$, $\eta_y = \eta \sin \theta_1$, $\xi_x = \xi \cos \theta_2$, $\xi_y = \xi \sin \theta_2$. The ranges of these angles are

$$0 \leq \phi \leq \pi/2, \quad 0 \leq \theta_1 \leq 2\pi, \quad 0 \leq \theta_2 \leq 2\pi .$$

To obtain the harmonics, in a manner which is suitable to also demonstrate the link with the KL harmonics, we introduce complex combinations of the Jacobi coordinates, i.e. the monomials

$$\begin{aligned} z_1 &= (\eta_x + i\eta_y) + i(\xi_x + i\xi_y) \\ z_1^* &= (\eta_x - i\eta_y) - i(\xi_x - i\xi_y) \\ z_2 &= (\eta_x - i\eta_y) + i(\xi_x - i\xi_y) \\ z_2^* &= (\eta_x + i\eta_y) - i(\xi_x + i\xi_y) \end{aligned} \tag{8}$$

It then follows that

$$\begin{aligned} \rho^2 &= \frac{1}{2}(z_1 z_1^* + z_2 z_2^*) \\ \nabla^2 &= 8\left(\frac{\partial^2}{\partial z_1 \partial z_1^*} + \frac{\partial^2}{\partial z_2 \partial z_2^*}\right), \end{aligned} \tag{9}$$

and, clearly, z_1 , z_1^* , z_2 and z_2^* each satisfies Laplace’s equation, as do the combinations $z_1 z_2$, $z_1 z_2^*$, $z_1^* z_2$, $z_1^* z_2^*$ and these combinations raised to integer powers.

Writing $\rho_1^2 = z_1 z_1^*$ and $\rho_2^2 = z_2 z_2^*$, we can write as the most general solution arising from the monomials z_1 and z_2 :

$$z_1^{l_1} z_2^{l_2} P_l^{l_2, l_1} \left(\frac{\rho_2^2 - \rho_1^2}{\rho_2^2 + \rho_1^2} \right) (\rho_1^2 + \rho_2^2)^l,$$

where l_1 , l_2 and l are positive integers or zero, and $P_l^{l_2, l_1}$ is a Jacobi polynomial.

In terms of the angles, our expression becomes proportional to:

$$\rho^{l_1+l_2+2l}(\cos^2 \phi)^{l_1/2}(\sin^2 \phi)^{l_2/2} P_l^{l_2, l_1}(\cos 2\phi) e^{i\theta_1 l_1} e^{i\theta_2 l_2}$$

and, finally, in terms of z equal to $\cos 2\phi$, we define our unnormalized harmonic:

$$Y_l^{l_1, l_2}(\theta_1, \theta_2, z) = (1+z)^{|l_1|/2} (1-z)^{|l_2|/2} P_l^{|l_2|, |l_1|}(z) e^{i\theta_1 l_1} e^{i\theta_2 l_2}, \quad (10)$$

where now l_1 and l_2 can be positive, negative, integers - or zero. (This takes into account the other combinations $z_1 z_2^*$, etc.) The order of the harmonic is N equal to $|l_1| + |l_2| + 2l$.

The Adiabatic Differential Equation

Writing

$$\nabla_\eta^2 + \nabla_\xi^2 = \left(\frac{\partial^2}{\partial \rho^2} + \frac{3}{\rho} \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \nabla_\Omega^2, \quad (11)$$

inserting our polar coordinates into the left hand side and changing to our variable z , we find:

$$\nabla_\Omega^2 = 4(1-z^2) \frac{\partial^2}{\partial z^2} - 8z \frac{\partial}{\partial z} + \frac{2}{(1+z)} \frac{\partial^2}{\partial \theta_1^2} + \frac{2}{(1-z)} \frac{\partial^2}{\partial \theta_2^2}. \quad (12)$$

If we now write our adiabatic eigenfunctions as

$$B_N^{l_1 l_2}(\rho, \Omega) = e^{il_1 \theta_1} e^{il_2 \theta_2} (1+z)^{|l_1|/2} (1-z)^{|l_2|/2} F_l^{|l_1|, |l_2|}(\rho, z), \quad (13)$$

then the functions F will satisfy the equation:

$$\begin{aligned} & \left[-4(1-z^2) \frac{\partial^2}{\partial z^2} + 4((2+l_1+l_2)z + l_2 - l_1) \frac{\partial}{\partial z} \right] F_l^{l_1, l_2}(\rho, z) \\ & + \left[(l_1 + l_2)(l_1 + l_2 + 2) + \rho^2 \bar{V}(\rho, z) \right] F_l^{l_1, l_2}(\rho, z) = \rho^2 \lambda(\rho) F_l^{l_1, l_2}(\rho, z) \end{aligned} \quad (14)$$

where $\bar{V}(\rho, z)$ equals $2m/\hbar^2$ times the potential and in our notation we have dropped the absolute value indications.

When $\bar{V}(\rho, z) = 0$, we can obtain a solution which is analytic between $-1 \leq z \leq +1$. For λ equal to $(l_1 + l_2 + 2l)(l_1 + l_2 + 2l + 2)/\rho^2$ and l a non-negative integer, we find that our F is simply $P_l^{l_2, l_1}(z)$, the Jacobi polynomial which appears in our Eq. (10). The N that appears in the B of Eq. (13) is the order of the corresponding harmonic.

For our potential

$$\bar{V}(\rho, z) = \begin{cases} (2m/\hbar^2) V_0 & -1 \leq z \leq -1 + 1/\rho^2 \\ 0 & -1 + 1/\rho^2 < z \leq 1, \end{cases} \quad (15)$$

the solutions of this equation which behave reasonably at z equal to -1 and $+1$ will be seen to be proportional to extensions of the Jacobi polynomials to functions with non-integer indices, in a relationship similar to that of Legendre polynomials and Legendre functions.

To motivate and clarify our procedure we first consider the case of $l_1 = l_2 = 0$, with and without potential.

When the potential is put to zero and we factor a 4 as well as change the sign, the differential equation reads

$$\left[(1 - z^2) \frac{\partial^2}{\partial z^2} - 2z \frac{\partial}{\partial z} + l(l+1) \right] F_l^{0,0}(\rho, z) = 0. \quad (16)$$

This is, of course, the Legendre differential equation and, with l a positive or zero integer, the well behaved solutions are the Legendre polynomials.

In the case of our potential, which is zero or a constant (only a function of ρ) in the different ranges of z , we can write our differential equation in a very similar form, i.e. as

$$\left[(1 - z^2) \frac{\partial^2}{\partial z^2} - 2z \frac{\partial}{\partial z} + \nu(\nu+1) \right] F_\nu^{0,0}(\rho, z) = 0, \quad (17)$$

where for $-1 + 1/\rho^2 < z \leq 1$

$$\nu(\nu+1) = \rho^2 \lambda(\rho)/4 \quad (18)$$

and for $-1 \leq z \leq -1 + 1/\rho^2$

$$\nu(\nu+1) = \rho^2 [\lambda(\rho) - \bar{V}_0]/4. \quad (19)$$

Denoting the respective values of ν as ν_1 and ν_2 , the corresponding solutions are the Legendre function $P_{\nu_1}(z)$ and the combination

$$P_{\nu_2}(-z) = \cos(\pi\nu_2) P_{\nu_2}(z) - (2/\pi) \sin(\pi\nu_2) Q_{\nu_2}(z),$$

of the first and second Legendre functions.

The point is as follows. Whereas $P_{\nu_1}(z)$ is well behaved at z equal to 1, and is suitable as a solution for its range in z from $-1 + 1/\rho^2$ to 1, both the $P_{\nu_2}(z)$ and $Q_{\nu_2}(z)$ have a logarithmic singularity at z equals -1 . The combination that we propose, however, is such that the logarithmic terms cancel out and the combination[4] is a well behaved solution in the range -1 to $-1 + 1/\rho^2$.

Expressing these solutions as power series, the first about $z = 1$, the second about $z = -1$, we obtain

$$\begin{aligned} & {}_2F_1(-\nu_1, \nu_1 + 1; 1; \tfrac{1}{2}(1 - z)), \quad \text{for } -1 + 1/\rho^2 < z \leq 1 \\ & \text{and} \\ & {}_2F_1(-\nu_2, \nu_2 + 1; 1; \tfrac{1}{2}(1 + z)), \quad \text{for } -1 \leq z \leq -1 + 1/\rho^2 \end{aligned} \quad (20)$$

Our overall solutions are then obtained by matching the logarithmic derivative of the two solutions (above) at the boundary: at z equal $-1 + 1/\rho^2$. This then also yields the adiabatic eigenvalues.

It now remains to note that for the cases of l_1 and l_2 not equal to zero, we can use the same procedure. We have, for the two regimes, solutions proportional to

$$\begin{aligned} & {}_2F_1(-\nu_1, \nu_1 + |l_1| + |l_2| + 1; |l_2| + 1; \tfrac{1}{2}(1 - z)), \quad \text{for } -1 + 1/\rho^2 < z \leq 1 \\ & \text{and} \\ & {}_2F_1(-\nu_2, \nu_2 + |l_1| + |l_2| + 1; |l_1| + 1; \tfrac{1}{2}(1 + z)), \quad \text{for } -1 \leq z \leq -1 + 1/\rho^2 \end{aligned} \quad (21)$$

For each choice of l_1 and l_2 there is an infinite set of values of ν_1 for which the logarithmic derivative of the hypergeometric functions can be matched at z equal to $-1 + 1/\rho^2$. For each such value of ν_1 , the adiabatic eigenvalue is then given by

$$\lambda(\rho) = \frac{(2\nu_1 + |l_1| + |l_2| + 1)^2 - 1}{\rho^2}. \quad (22)$$

When $V_0 = 0$, the adiabatic basis reduces to the hyperspherical harmonic basis of Eqn. (10), since the hypergeometric functions reduce to Jacobi polynomials, and $\nu_1 \equiv \nu_2 = l$. So our $B_N^{l_1, l_2}$ is precisely the $Y_l^{l_1, l_2}(\theta_1, \theta_2, z)$.

Comparison of the Adiabatic Eigenvalues

When the numerical work was done (using the KL basis), lists were made of the appropriate harmonics needed to form the matrices (potential and centrifugal) which, when added and diagonalized, yield the adiabatic eigenvalues. We now need to identify these eigenvalues and compare them with those obtained by the new method. This is not trivial, but an immediate remark can be made.

First of all, the angular momentum λ is a good quantum number, with

$$\lambda = l_1 + l_2. \quad (23)$$

This follows from the fact that l_1 specifies the angular momentum of the 1-2 pair and l_2 specifies the angular momentum of the third particle relative to the center of mass of the first two. Thus their sum defines the total inplane angular momentum. Hence, for example, when $\lambda = 0$ we can have all pairs l_1 and l_2 with $l_1 = -l_2$. If $l_1 = l_2 = 0$, this then provides a single eigenvalue for each choice of $N = 2l$, $l = 0, 1, 2, \dots$.

Another indicator is whether n is even or odd, which is very significant in the drawing up of the lists, associated with the symmetries of the harmonics. Proceeding, then, we compare values of the effective potential, defined by

$$V(\rho, N) = \lambda(\rho) - \frac{(N+1)^2 - \frac{1}{4}}{\rho^2}, \quad (24)$$

where we subtract from each eigenvalue the value of the centrifugal term that would correspond to it, if the binary potential were allowed to go to zero. These have been extensively tabulated by Zhen[5].

Table 1 compares the results in the simplest case, $N = 0$, where we demonstrate the convergence of the truncated matrix method with the result obtained directly, for a sample value of $\rho = 5$ and $\Lambda^* = 10$. ($\Lambda^* = (h^2/mV_0\sigma^2)^{1/2}$)

N_{max}	$V(5, 0)$
110	0.011754744
120	0.011754730
130	0.011754670
140	0.011754666
Direct	0.011754562

Table 1. Convergence of the matrix method

A more extensive set of comparisons is made in *Table 2*, where selected values of the effective potential, obtained from eigenvalues of the truncated matrix, are chosen for various values of N , λ and n and compared with the direct results. In all cases, except the first, the matrix was truncated at $N_{max} = 100$.

$V(\rho, N)$							
<i>Truncated Matrix</i>				<i>Direct</i>			
n	λ	N	$V(5, N)$	l	$ l_1 $	$ l_2 $	$V(5, N)$
E	0	0	0.011754666	0	0	0	0.011754562
E	0	2	0.037577818	1	0	0	0.037577462
O	0	2	0.000874927	0	1	1	0.000874911
E	0	4	0.062609805	2	0	0	0.062609219
E	0	4	0.00005971	0	2	2	0.00005971
O	2	4	0.00413519	1	1	1	0.00413512
E	1	1	0.024168	0	0	1	0.02416738
E	1	1	0.00029592	0	1	0	0.00029591
O	1	3	0.000024	0	2	1	0.00002426
O	1	3	0.00172537	0	1	2	0.00172529
E	1	3	0.050462	1	0	1	0.0504588
E	1	3	0.00226748	1	1	0	0.00226737
E	2	2	0.00000616	0	2	0	0.00000616
O	2	2	0.036849	0	0	2	0.03684737
E	2	4	0.000088636	1	2	0	0.000088629
E	4	4	0.062866	1	0	2	0.06286247

Table 2. Some effective potential values in the “delta-bar” class

Asymptotic Behaviour

The matching of logarithmic derivatives provides a means of obtaining information about the asymptotic behaviour of the eigenvalues, and hence the effective potentials, as the hyper-radius, ρ , gets large. There is however a particular difficulty in finding this behaviour. It is that it is not simply a case of looking at the limiting behaviour of ${}_2F_1(a, b; c; \epsilon)$ and ${}_2F_1(a, b; c; 1 - \epsilon)$ as $\epsilon \rightarrow 0$, because the expressions corresponding to a and b both depend on ρ .

In the simplest case, corresponding to $l_1 = l_2 = l = 0$, we find

$$\begin{aligned} \rho^2 V_{\text{eff}}(\rho, N) &= 4(N+1)\epsilon_0 \\ &\sim \frac{1}{\mathcal{A} + \mathcal{B} \ln \rho}, \end{aligned} \quad (25)$$

where

$$\mathcal{A} = \frac{I_0(\sqrt{2A})}{2(N+1)\sqrt{2A}I_1(\sqrt{2A})} + \frac{1}{4(N+1)} \ln 2 \quad (26)$$

and

$$\mathcal{B} = \frac{1}{2(N+1)} . \quad (27)$$

The I_i 's being modified Bessel functions of integer order of the first kind.

The next simplest case is with only $l_1 = 0$. Then

$$\mathcal{A} = \frac{1}{(N+1)} \left[\frac{I_0(\sqrt{2A})}{2\sqrt{2A}I_1(\sqrt{2A})} + \frac{1}{4} \ln 2 - \frac{1}{4} \sum_{p=1}^k \frac{1}{p} - \frac{1}{4} \sum_{q=1}^{k+m} \frac{1}{q} \right] \quad (28)$$

and

$$\mathcal{B} = \frac{1}{2(N+1)} , \quad (29)$$

where it should be understood that $\Sigma_1^0 \equiv 0$.

The case with $l_1 \neq 0$ introduces considerable complications, particularly to the form of \mathcal{A} , with higher order Bessel functions occurring, and so is not listed. However the expression for \mathcal{B} is exactly the same. This confirms the value postulated by Larsen [1].

It is impressive how well Zhen [5] did working with approximate values for the eigenvalues. In her thesis she compares her \mathcal{B} 's with the postulated values. If we compare her \mathcal{A} 's with the above expressions (see *Table 3*), we see just how consistent her calculations are.

N	l	l_2	\mathcal{A} (Zhen)	\mathcal{A} (here)
0	0	0	2.6064	2.8293
2	1	0	0.7581	0.7764
4	2	0	0.4146	0.4159
1	0	1	1.2381	1.2897
3	1	1	0.5493	0.5511
5	2	1	0.3356	0.3327

Table 3. Comparison of numerical and analytic asymptotic leading terms.

Thus, the conclusions previously obtained by assuming this form of asymptotic behaviour [2] are verified; at least in the “delta-bar” case.

Conclusion

It is now clear that the extensive numerical calculations of Zhen [5], using the truncated matrix approach, provided good estimates of the eigenvalues, the effective potentials, and the $2 + 1$ phase shifts of the third cluster. The results are consistent for the entire range of values of ρ , taking into consideration the requirement for larger N_{max} at larger values of ρ .

We were also able to demonstrate the all important logarithmic behaviour in the asymptotic form of some of the effective potentials. This insures that the corresponding phase shifts (dominant at low energies) go to zero, as the wave number goes to zero. For the other $2 + 1$ phase shifts, characterized by other group classifications of the harmonics, we can demonstrate by explicit calculations that both the asymptotic form of the effective potentials and the phase shifts go to zero in a stronger manner.

We would love to obtain similar asymptotic expressions for the effective potentials of the fully interacting problem. If we were able to do this, it would simplify enormously the cluster calculations, as well as increase its accuracy.

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